

On maximum Estrada indices of bipartite graphs with some given parameters*

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Abstract

The Estrada index of a graph G is defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i}$, where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of the adjacency matrix of G . In this paper, we characterize the unique bipartite graph with maximum Estrada index among bipartite graphs with given matching number and given vertex-connectivity, edge-connectivity, respectively.

Keywords: Estrada index; walk; maximum matching; vertex cut; connectivity

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1 Introduction

Let G be a simple graph on n vertices. The eigenvalues of G are the eigenvalues of its adjacency matrix, which are denoted by $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. The Estrada index of G , put forward by Estrada [7], is defined as

$$EE(G) = \sum_{i=1}^n e^{\lambda_i}.$$

The Estrada index has multiple applications in a large variety of problems, for example, it has been successfully employed to quantify the degree of folding of long-chain molecules,

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especially proteins [8, 9, 10], and it is a useful tool to measure the centrality of complex (reaction, metabolic, communication, social, etc.) networks [11, 12]. There is also a connection between the Estrada index and the extended atomic branching of molecules [13]. Besides these applications, the Estrada index has also been extensively studied in mathematics, see [16, 18, 20, 21, 22]. Ilić and Stevanović [16] obtained the unique tree with minimum Estrada index among the set of trees with a given maximum degree. Zhang, Zhou and Li [20] determined the unique tree with maximum Estrada indices among the set of trees with a given matching number. In [4], Du and Zhou characterized the unique unicyclic graph with maximum Estrada index. Wang et al. [19] determined the unique graph with maximum Estrada index among bicyclic graphs with fixed order, and Zhu et al. [23] determined the unique graph with maximum Estrada index among tricyclic graphs with fixed order. More mathematical properties on the Estrada index can be founded in [14].

A graph is bipartite if its vertex set can be partitioned into two subsets X and Y so that every edge has one end in X and the other end in Y . We denote a bipartite graph G with bipartition (X, Y) by $G[X, Y]$. If $G[X, Y]$ is simple and every vertex in X is joined to every vertex in Y , then G is called a complete bipartite graph. Up to isomorphism, there is a unique complete bipartite graph with parts of sizes m and n , denoted $K_{m,n}$. For an edge subset A of the complement of G , we use $G + A$ to denote the graph obtained from G by adding the edges in A .

A matching in a graph is a set of pairwise nonadjacent edges. If M is a matching, the two ends of each edge of M are said to be matched under M , and each vertex incident with an edge of M is said to be covered by M . A maximum matching is one which covers as many vertices as possible. The number of edges in a maximum matching of a graph G is called the matching number of G and denoted by $\alpha'(G)$. Let $\mathcal{M}_{n,p}$ be the set of bipartite graphs on n vertices with $\alpha'(G) = p$.

A cut vertex(edge) of a graph is a vertex(edge) whose removal increases the number of components of the graph. A(An) vertex(edge) cut of a graph is a set of vertices(edges) whose removal disconnects the graph. The connectivity(edge-connectivity) of a graph G is defined as

$$\kappa(G) = \min\{|G|-1, |S| : S \text{ is a vertex cut of } G\}, \kappa'(G) = \min\{|S| : S \text{ is an edge cut of } G\}.$$

Let $\mathcal{C}_{n,s}(\mathcal{D}_{n,s})$ denote the set of bipartite graphs on n vertices with $\kappa(G) = s(\kappa'(G) = s)$. For other undefined terminology and notation we refer to Bondy and Murty [1].

In [5], Du, Zhou and Xing determined the graphs with maximum Estrada indices among graphs with given number of cut vertices, connectivity, and edge connectivity,

respectively. In this paper, we consider bipartite graphs, and characterize the unique bipartite graph with maximum Estrada indices among $\mathcal{M}_{n,p}$, $\mathcal{C}_{n,s}$ and $\mathcal{D}_{n,s}$, respectively.

2 Preliminaries

Denote by $M_k(G)$ the k -th spectral moment of a graph G , i.e., $M_k(G) = \sum_{i=1}^n \lambda_i^k$. It is well-known [3] that $M_k(G)$ is equal to the number of closed walks of length k in G . Then

$$EE(G) = \sum_{i=1}^n \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!} = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \quad (1)$$

For n -vertex graphs G_1 and G_2 , if $M_k(G_1) \leq M_k(G_2)$ for all positive integers k , then by Eq.(1) we have that $EE(G_1) \leq EE(G_2)$ with equality if and only if $M_k(G_1) = M_k(G_2)$ for all positive integers k .

Let k be a positive integer. For $u, v \in V(G)$, let $W_k(G; u, v)$ denote the set of (u, v) -walks of length k in G , and let $M_k(G; u, v) = |W_k(G; u, v)|$. For convenience, let $W_k(G; u) = W_k(G; u, u)$ and $M_k(G; u) = M_k(G; u, u)$.

For graphs G_1 and G_2 with $u_1, v_1 \in V(G_1)$ and $u_2, v_2 \in V(G_2)$, if $M_k(G_1; u_1, v_1) \leq M_k(G_2; u_2, v_2)$ for all positive integers k , then we write $(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$, and if $(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$ and there is a positive integer k_0 such that $M_{k_0}(G_1; u_1, v_1) < M_{k_0}(G_2; u_2, v_2)$, then we write $(G_1; u_1, v_1) \prec (G_2; u_2, v_2)$. For convenience, we write $(G_1; u_1) \preceq (G_2; u_2)$ for $(G_1; u_1, u_1) \preceq (G_2; u_2, u_2)$, and $(G_1; u_1) \prec (G_2; u_2)$ for $(G_1; u_1, u_1) \prec (G_2; u_2, u_2)$.

Lemma 2.1 [15] *Let G be a graph. Then for any edge $e \notin E(G)$, one has $EE(G + e) > EE(G)$.*

Lemma 2.2 [14] *If a graph G is bipartite, and if n_0 is the nullity (=the multiplicity of its eigenvalue zero) of G , then*

$$EE(G) = n_0 + 2 \sum_{+} \cosh(\lambda_i), \quad (2)$$

where \cosh stands for the hyperbolic cosine [$\cosh(x) = (e^x + e^{-x})/2$], whereas \sum_{+} denotes summation over all positive eigenvalues of the corresponding graph.

As is well known [2] that the spectrum of a complete bipartite graph K_{n_1, n_2} is $\sqrt{n_1 n_2}$, $-\sqrt{n_1 n_2}$, $0(n_1 + n_2 - 2 \text{ times})$. By the definition, we have

Lemma 2.3 [14]

$$EE(K_{n_1, n_2}) = n_1 + n_2 - 2 + 2\cosh(\sqrt{n_1 n_2}).$$

By the monotonicity of $f(x) = \cosh(x)$, it is obvious that

Corollary 2.4

$$EE(K_{1, n-1}) < EE(K_{2, n-2}) < \dots < EE(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}). \quad (3)$$

Lemma 2.5 *Let G be a non-trivial graph with $u, v \in V(G)$ such that $N_G(u) = N_G(v)$. Then for any $k \geq 0$, one has*

$$M_k(G; u) = M_k(G; v) = M_k(G; u, v) = M_k(G; v, u).$$

Proof. For any walk $W \in W_k(G; u, u)$, let $f(W)$ be the walk obtained from W by replacing its first and last vertex u by v . This is practical since $N_G(u) = N_G(v)$. Obviously, $f(W) \in W_k(G; v, v)$ and f is a bijection from $W_k(G; u, u)$ to $W_k(G; v, v)$, and so $M_k(G; u) = M_k(G; v)$. We can similarly construct a bijection from $W_k(G; u, u)$ to $W_k(G; u, v)$ or $W_k(G; v, u)$. So we have

$$M_k(G; u) = M_k(G; v) = M_k(G; u, v) = M_k(G; v, u),$$

as desired. ■

Lemma 2.6 *Let K_{n_1, n_2} be the complete bipartite graph with $X = \{x_1, x_2, \dots, x_{n_1}\}$ and $Y = \{y_1, y_2, \dots, y_{n_2}\}$. For any $k > 0$, one has that for any $1 \leq i, j \leq n_1$ and $1 \leq r, s \leq n_2$,*

$$M_{2k}(G; x_i, x_j) = n_1^{k-1} n_2^k, \quad M_{2k}(G; y_r, y_s) = n_2^{k-1} n_1^k. \quad (4)$$

Furthermore, $M_{2k}(G) = 2(n_1 n_2)^k$.

Proof. Let $W = u_1(= x_i)u_2 \dots u_{2k}u_{2k+1}(= x_j) \in W_{2k}(G; x_i, x_j)$ be an (x_i, x_j) -walk of length $2k$. Since G is a complete bipartite graph, it is straightforward that $u_{2r+1} \in \{x_1, x_2, \dots, x_{n_1}\}$ and $u_{2r} \in \{y_1, y_2, \dots, y_{n_2}\}$ for $r = 1, 2, \dots, (k-1)$. Moreover, we know that each u_{2r-1} can be arbitrarily chosen from X and each u_{2r} can be arbitrarily chosen from Y . Hence, for fixed x_i and x_j there are $n_1^{k-1} n_2^k$ walks of length $2k$ between them, that is, $M_{2k}(G; x_i, x_j) = n_1^{k-1} n_2^k$ for any $1 \leq i, j \leq n_1$. Similarly, we can obtain $M_{2k}(G; y_t, y_r) = n_2^{k-1} n_1^k$ for any $1 \leq t, r \leq n_2$. By the definition of $W_{2k}(G)$, we have

$$M_{2k}(G) = \sum_{i=1}^{n_1} M_{2k}(G; x_i) + \sum_{j=1}^{n_2} M_{2k}(G; y_j) = 2(n_1 n_2)^k.$$

The proof is complete. ■

Let $S_1 = \{v_1, v_2, \dots, v_s\}$ be an independent set of G_1 and $S_2 = \{u_1, u_2, \dots, u_s\}$ an independent set of G_2 . We denote $G_1 \cup_s G_2$ as the graph obtained from G_1 and G_2 by identifying v_i with u_i for each i ($1 \leq i \leq s$). We denote the identified vertex set in $G_1 \cup_s G_2$ by S . Likewise, we can also get $G'_1 \cup_s G'_2$ from G'_1 and G'_2 , where the two independent sets that should be identified are $S'_1 = \{v'_1, v'_2, \dots, v'_s\}$ and $S'_2 = \{u'_1, u'_2, \dots, u'_s\}$, respectively.

Lemma 2.7 *Let $G = G_1 \cup_s G_2$ and $G' = G'_1 \cup_s G'_2$ be the graphs of order n defined as above satisfying the following conditions:*

1. For any $k > 0$,

$$M_k(G_1) \leq M_k(G'_1), \quad M_k(G_2) \leq M_k(G'_2); \quad (5)$$

2. For any $1 \leq i, j \leq s$,

$$(G_1; v_i, v_j) \preceq (G'_1; v'_i, v'_j), \quad (G_2; u_i, u_j) \preceq (G'_2; u'_i, u'_j). \quad (6)$$

Then for any $k > 0$, $M_k(G) \leq M_k(G')$. Furthermore, $EE(G) \leq EE(G')$, with equality holds if and only if all the equalities in (5) and (6) hold.

Proof. For any $k > 0$, let $W_k(G)$ denote the set of closed walks of length k in G , we can see that

$$W_k(G) = W_k(G_1) \cup W_k(G_2) \cup W_k^3(G), \quad (7)$$

where $W_k^3(G)$ is the set of closed walks of length k in G containing both vertices in $G_1 \setminus S_1$ and vertices in $G_2 \setminus S_2$. Similarly, one has

$$W_k(G') = W_k(G'_1) \cup W_k(G'_2) \cup W_k^3(G'), \quad (8)$$

where $W_k^3(G')$ is the set of closed walks of length k in G' containing both vertices in $G'_1 \setminus S'_1$ and vertices in $G'_2 \setminus S'_2$.

By (5), we know that $|W_k(G_1)| \leq |W_k(G'_1)|$ and $|W_k(G_2)| \leq |W_k(G'_2)|$. We only need to show that $|W_k^3(G)| \leq |W_k^3(G')|$. In fact, there exists an injection from $W_k^3(G)$ to $W_k^3(G')$. In the following, we will construct such an injection.

For any $1 \leq i, j \leq s$, by (6) we know that for any $l > 0$,

$$M_l(G_1; v_i, v_j) \leq M_l(G'_1; v'_i, v'_j), \quad M_l(G_2; u_i, u_j) \leq M_l(G'_2; u'_i, u'_j). \quad (9)$$

So there exist an injection $f_{i,j}^l$ from $W_l(G_1; v_i, v_j)$ to $W_l(G'_1; v'_i, v'_j)$, and an injection $g_{i,j}^l$ from $W_l(G_2; u_i, u_j)$ to $W_l(G'_2; u'_i, u'_j)$ for any $1 \leq i, j \leq s$ and any $l > 0$. We will omit the subscript of $f_{i,j}^l$ and $g_{i,j}^l$ if there is no confusion about the first and last vertices of the walks we considered.

For any $W \in W_k^3(G)$, we call a maximal G_1 walk of W a 1-block, and a maximal G_2 walk of W a 2-block. From the definition, we have that the ends of a 1-block and a 2-block are both contained in S . Since $W_k^3(G)$ is the set of closed walks of length k in G_1 and contains both vertices in $G_1 \setminus S_1$ and vertices in $G_2 \setminus S_2$, there exist at least one 1-block and one 2-block, and the 1-blocks and 2-blocks appear one by one alternately with equal number. Hence we can decompose W as follows:

$$W = (B_0)B_1B_2B_3B_4 \dots B_r, \text{ where } r \text{ is even(odd),}$$

where B_{2i-1} is a 1-block of length l_{2i-1} , and B_{2i} is a 2-block of length l_{2i} . We define a map φ from $W \in W_k^3(G)$ to $W \in W_k^3(G')$ as follows:

$$\varphi(W) = (g^{l_0}(B_0))f^{l_1}(B_1)g^{l_2}(B_2)f^{l_3}(B_3)g^{l_4}(B_4) \dots$$

Then $\varphi(W)$ is a closed walk in $W \in W_k^3(G')$. Since both $f_{i,j}^l$ and $g_{i,j}^l$ are injection, we can easily deduce that φ is an injection. Thus, $|W_k^3(G)| \leq |W_k^3(G')|$, with equality holds if and only if for any $1 \leq i, j \leq s$ and any $l > 0$, $f_{i,j}^l$ and $g_{i,j}^l$ are bijections, that is, all the qualities in (6) hold. Hence, we have

$$\begin{aligned} M_k(G) &= |W_k(G_1)| + |W_k(G_2)| + |W_k^3(G)| \\ &\leq |W_k(G'_1)| + |W_k(G'_2)| + |W_k^3(G')| \\ &= M_k(G'). \end{aligned}$$

Therefore, the result follows. ■

3 Maximum Estrada index of bipartite graphs with a given matching number

A covering of a graph G is a vertex subset $K \subseteq V(G)$ such that each edge of G has at least one end in the set K . The number of vertices in a minimum covering of a graph G is called the covering number of G and denoted by $\beta(G)$.

Lemma 3.1 (The König-Egerváry Theorem, [6, 17]). *In any bipartite graph, the number of edges in a maximum matching is equal to the number of vertices in a minimum covering.*

Let $G = G[X, Y]$ be a bipartite graph such that $G \in \mathcal{M}_{n,p}$. From Lemma 3.1, we know that $\beta(G) = p$. Let S be a minimum covering of G and $X_1 = S \cap X$, $Y_1 = S \cap Y$. Without loss of generality, suppose that $|X_1| \geq |Y_1|$ in the following analysis. Set $X_2 = X \setminus X_1$, $Y_2 = Y \setminus Y_1$. We have that $E(X_2, Y_2) = \emptyset$ since S is a covering of G .

Let $G^*[X, Y]$ be a bipartite graph with the same vertex set as G such that $E(G^*) = \{xy : (x \in X_1, y \in Y) \text{ or } (x \in X_2, y \in Y_1)\}$. Obviously, G is a subgraph of G^* . From Lemma 2.1, we know that

$$EE(G) \leq EE(G^*), \quad (10)$$

with equality holds if and only if $G \cong G^*$. Let

$$G^{**} = G^* - \{uv : u \in X_2, v \in Y_1\} + \{uw : u \in X_2, w \in X_1\},$$

Then we have the following conclusion:

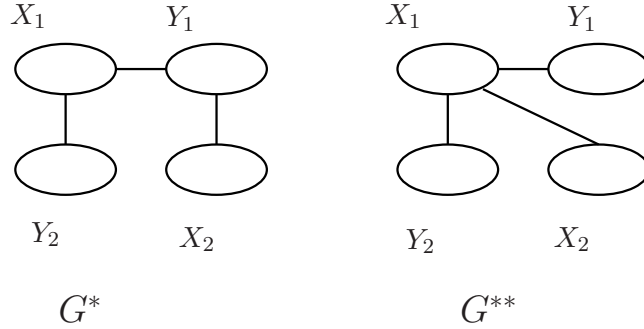


Figure 1. G^* and G^{**}

Lemma 3.2 *Let G^* and G^{**} be the graph defined above (see Figure 1). Then one has*

$$EE(G^*) \leq EE(G^{**}), \quad (11)$$

with equality holds if and only if $G^ \cong G^{**}$.*

Proof. Let $G_1 = G^*[X_1 \cup Y_2]$, $G_2 = G^*[X \cup Y_1]$, and $G'_1 = G^{**}[X_1 \cup Y_2]$, $G'_2 = G^{**}[X \cup Y_1]$. We can see that $G_1 = G'_1$, $G_2 \cong K_{|X_1|+|X_2|, |Y_1|}$ and $G'_2 \cong K_{|X_1|, |Y_1|+|X_2|}$. Furthermore, $G^* = G_1 \cup_{|X_1|} G_2$, and $G^{**} = G'_1 \cup_{|X_1|} G'_2$ with $S_1 = S_2 = S'_1 = S'_2 = X_1 = \{x_1, x_2, \dots, x_{|X_1|}\}$.

By Lemma 2.6, we have

$$M_{2k}(G_2) = 2(|X_1| + |X_2|)^k |Y_1|^k, \quad M_{2k}(G'_2) = 2|X_1|^k (|X_2| + |Y_1|)^k.$$

Since $|X_1| \geq |Y_1|$, we have $M_{2k}(G_2) \leq M_{2k}(G'_2)$. Furthermore, as both G_2 and G'_2 are bipartite graphs, one has $M_{2k-1}(G_2) = M_{2k-1}(G'_2) = 0$ for any $k > 0$. Now condition 1 of Lemma 2.7 is satisfied.

For any $x_i, x_j \in X_1$, by Lemma 2.6 we know that for any $l > 0$,

$$\begin{aligned} M_{2l}(G_2; x_i, x_j) &= (|X_1| + |X_2|)^{l-1} |Y_1|^l = |Y_1|(|X_1| + |X_2|)^{l-1} |Y_1|^{l-1}, \\ M_{2l}(G'_2; x_i, x_j) &= |X_1|^{l-1} (|X_2| + |Y_1|)^l = (|X_2| + |Y_1|)(|X_1|)^{l-1} (|X_2| + |Y_1|)^{l-1}. \end{aligned}$$

As $|X_1| \geq |Y_1|$, we have $(|X_1| + |X_2|)|Y_1| \leq |X_1|(|X_2| + |Y_1|)$. Hence

$$M_{2l}(G_2; x_i, x_j) \leq M_{2l}(G'_2; x_i, x_j),$$

with equality holds if and only if $|X_2| = 0$. Together with $M_{2l-1}(G_2; x_i, x_j) = M_{2l-1}(G'_2; x_i, x_j) = 0$, condition 2 of Lemma 2.7 is satisfied. So we have $EE(G^*) \leq EE(G^{**})$, with equality holds if and only if $|X_2| = 0$, i.e., $G^* \cong G^{**}$. ■

By (10) and (11), together with Corollary 2.4, it is straightforward to see that

Theorem 3.3 *Among the graphs in $\mathcal{M}_{n,p}$, $K_{p,n-p}$ is the unique graph with maximum Estrada index.*

4 Maximum Estrada index of bipartite graphs with a given connectivity(resp. edge connectivity)

For two complete bipartite graphs K_{n_1, n_2} and K_{m_1, m_2} , we define a graph $O_s \vee_1$ ($K_{n_1, n_2} \cup K_{m_1, m_2}$), where \cup is the union of two graphs, O_s ($s \geq 1$) is an empty graph of order s and \vee_1 is a graph operation that joins all the vertices in O_s to the vertices belonging to the partitions of cardinality n_1 in K_{n_1, n_2} and m_1 in K_{m_1, m_2} (see Figure. 2), respectively.

Lemma 4.1 *For an n -vertex bipartite graph $O_s \vee_1 (K_1 \cup K_{p,q})$ with $p < q + s$ and $q \geq 0$, one has $EE(O_s \vee_1 (K_1 \cup K_{p,q})) < EE(O_s \vee_1 (K_1 \cup K_{q+s, p-s}))$.*

Proof. Let us denote $O_s \vee_1 (K_1 \cup K_{p,q})$ by G and $O_s \vee_1 (K_1 \cup K_{q+s, p-s})$ by G' .

Let $G_1 = G[\{u\} \cup O_s]$, $G_2 = G - \{u\}$, we can see that $G = G_1 \cup_s G_2$. Similarly, let $G'_1 = G'[\{u\} \cup O_s]$, $G'_2 = G' - \{u\}$, then $G' = G'_1 \cup_s G'_2$.

It is obvious that $G_1 \cong G'_1 \cong K_{1,s}$, $G_2 \cong K_{s+q, p}$ and $G'_2 \cong K_{s+p-s, q+s}$. Thus for any $k > 0$, $M_k(G_1) = M_k(G'_1)$ and for any $1 \leq i, j \leq s$, $(G_1; a_i, a_j) \preceq (G'_1; a_i, a_j)$. From Lemma 2.6, we know that $M_k(G_2) = M_k(G'_2)$ for any $k > 0$.

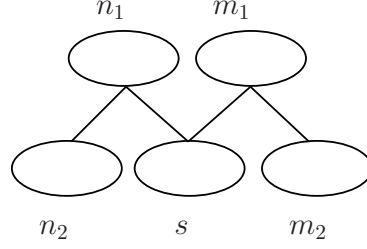


Figure 2. $O_s \vee_1 (K_{n_1, n_2} \cup K_{m_1, m_2})$

Moreover, by Lemma 2.6 we have that for any $k > 0$ and $1 \leq i, j \leq s$,

$$M_{2k}(G_2; a_i, a_j) = (s + q)^{k-1} p^k < (s + q)^k p^{k-1} = M_{2k}(G'_2; a_i, a_j).$$

Together with $M_{2k-1}(G_2; a_i, a_j) = 0 = M_{2k-1}(G'_2; a_i, a_j)$, we have $(G_2; a_i, a_j) \prec (G'_2; a_i, a_j)$. Hence, by Lemma 2.7 we have $EE(G) < EE(G')$, as desired. ■

Lemma 4.2 *For an n -vertex bipartite graph $O_s \vee_1 (K_1 \cup K_{p,q})$ with $p > q + s + 1$ and $q > 0$, one has $EE(O_s \vee_1 (K_1 \cup K_{p,q})) < EE(O_s \vee_1 (K_1 \cup K_{p-1, q+1}))$.*

Proof. Let $X = (x_1, x_2, \dots, x_n)^T$ be an eigenvector of $O_s \vee_1 (K_1 \cup K_{p,q})$ corresponding to the eigenvalue λ . By the eigenvalue-equations, for any $i = 1, 2, \dots, n$,

$$\lambda x_i = \sum_{j: v_i v_j \in E(O_s \vee_1 (K_1 \cup K_{p,q}))} x_j.$$

Thus, for any eigenvalue of $O_s \vee_1 (K_1 \cup K_{p,q})$ with $\lambda \neq 0$, one has $x_i = x_j$ if $N(v_i) = N(v_j)$. So, we know that the eigenvalue of $O_s \vee_1 (K_1 \cup K_{p,q})$ which is not equal to 0 satisfies:

$$\begin{cases} \lambda x_1 = s x_2, \\ \lambda x_2 = x_1 + p x_3, \\ \lambda x_3 = s x_2 + q x_4, \\ \lambda x_4 = p x_3. \end{cases} \quad (12)$$

As the root of (12) is also the root of

$$\lambda^4 - \lambda^2(s + pq + ps) + pqs = 0, \quad (13)$$

then we have that

$$EE(G) = n - 4 + 2\cosh(x_1) + 2\cosh(x_2),$$

where x_1, x_2 are the different positive roots of (13). We may assume that $r = x_1 > x_2$ and $k = x_1 x_2 = \sqrt{pq s}$. Then $r > \sqrt{k} > 0$, and we can get

$$EE(O_s \vee_1 (K_1 \cup K_{p,q})) = f(r, k) = n - 4 + 2\cosh(r) + 2\cosh(k/r). \quad (14)$$

Then we have

$$\frac{\partial f(r, k)}{\partial r} = (e^r - e^{-r}) - \frac{k}{r^2}(e^{k/r} - e^{-k/r}) > 0, \quad (15)$$

and

$$\frac{\partial f(r, k)}{\partial k} = \frac{1}{r}(e^{k/r} - e^{-k/r}) > 0. \quad (16)$$

Let $k' = \sqrt{(p-1)(q+1)s}$. As $pqs - (p-1)(q+1)s = s(q+1-p) < 0$, we have $k < k'$.

On the other hand, let

$$g(x, p, q, s) = x^4 - x^2(s + pq + ps) + pqs,$$

and r' be the maximum root of $g(x, p-1, q+1, s)$, we will show $r' > r$. In fact, as $g(r, p, q, s) - g(r, p-1, q+1, s) = (p-q-s-1)r^2 - (p-s-1)s \geq r^2 - (p-s-1)s > 0$, we have $g(r, p-1, q+1, s) < 0$. Together with $g(\infty, p-1, q+1, s) > 0$, we can get $r' > r$. Thus, by (15) and (16) we have $f(r, k) < f(r', k')$, i.e., $EE(O_s \vee_1 (K_1 \cup K_{p,q})) < EE(O_s \vee_1 (K_1 \cup K_{p-1, q+1}))$. ■

Lemma 4.3 For $s \leq \lceil \frac{n-1}{2} \rceil - 1$, one has $EE(K_{s, n-s}) < EE(O_s \vee_1 (K_1 \cup K_{n-s-2, 1}))$.

Proof. By Lemma 2.3, we have $EE(K_{s, n-s}) = n - 2 + 2\cosh(\sqrt{s(n-s)})$. As in the proof of Lemma 4.2, one has

$$EE(O_s \vee_1 (K_1 \cup K_{n-s-2, 1})) = n - 4 + 2\cosh(x_1) + 2\cosh(x_2),$$

where x_1 and x_2 are the different positive roots of $f(x) = 0$, where

$$f(x) = x^4 - x^2(s + (n-s-2) + (n-s-2)s) + (n-s-2)s.$$

Without loss of generality, we assume that $x_1 > x_2$. Then we have

$$\begin{aligned} f(\sqrt{s(n-s)}) &= -s(n^2 - 3ns - 3n + 2s^2 + 3s + 2) \\ &= -s((n-2s-3)(n-s) + 2) < 0, \end{aligned}$$

where the “ $<$ ” holds since $s \leq \lceil \frac{n-1}{2} \rceil - 1$, i.e., $n \geq 2s + 3$. Together with $f(\infty) > 0$, we have $x_1 > \sqrt{s(n-s)}$.

Now $x_1 > \sqrt{s(n-s)}$, $x_2 > 0$, then by the monotonicity of $\cosh(x)$, one has $\cosh(x_1) > \cosh(\sqrt{s(n-s)})$ and $\cosh(x_2) > 1$. We then deduce

$$EE(K_{s,n-s}) < EE(O_s \vee_1 (K_1 \cup K_{n-s-2,1})),$$

as desired. ■

Lemma 4.4 *Let G be a graph with maximum Estrada index in $\mathcal{C}_{n,s}$ and U be a minimum vertex cut. If $G - U$ has a nontrivial component G_1 , then $G - U$ has exactly two components, and the other component which is distinct from G_1 cannot be nontrivial.*

Proof. Let G_1, G_2, \dots, G_k be the components of $G - U$. Suppose $k \geq 3$. Then, we can add some appropriate edges in G between G_1, G_2, \dots, G_{k-1} so that the resulting graph G' is still bipartite. It is obvious that $G' \in \mathcal{C}_{n,s}$. By Lemma 2.1, we have $EE(G') > EE(G)$. This contradicts the fact that G has the maximum Estrada index among graphs in $\mathcal{C}_{n,s}$, and so we have $k = 2$.

If both G_1 and G_2 are nontrivial with bipartition (A, B) and (C, D) , respectively. Let $U = U_1 \cup U_2$ be the bipartition of U induced by the bipartition of G . Now joining all possible edges between the vertices of A and B , C and D , and U_1 and U_2 , we get a graph \widehat{G} in $\mathcal{C}_{n,s}$ such that $EE(\widehat{G}) \geq EE(G)$. Therefore, we assume $G = \widehat{G}$; see Figure 3. Suppose that G_1 and G_2 are the two nontrivial components of $G - U$. The bipartition of G_1 is (A, B) and the bipartition of G_2 is (C, D) . Let $U = U_1 \cup U_2$ be the bipartition of U induced by the bipartition of G . Now joining all possible edges between the vertices of A and B , C and D , and U_1 and U_2 , we get a graph \widehat{G} in $\mathcal{C}_{n,s}$ such that $EE(\widehat{G}) \geq EE(G)$. Therefore, we assume $G = \widehat{G}$; see Figure 3.

If there exists some vertex w in $G - U$ such that $d_G(w) = s$, then forming a complete bipartite graph within the vertices of $G \setminus w$ we would get a graph in $\mathcal{C}_{n,s}$ with larger Estrada index. Thus, we may assume that each vertex in $G - U$ has a degree greater than s . Let $|A| = m_1$, $|B| = m_2$, $|C| = n_1$, $|D| = n_2$, $|U_1| = t$, $|U_2| = k$.

We choose a vertex u_0 from C and observe that $d_G(u_0) = t + |D| > s$, where t ($0 \leq t \leq s$) is the total number of edges joining u_0 and the vertices of U_1 . Note that $U_1 \cup U_2$ is the vertex cut of order s , hence $m_1, n_1 > t$, $m_2, n_2 > k$. Without loss of generality, we may assume that $m_1 = \max\{m_1, m_2, n_1, n_2\}$ and note that $s \geq 1$, hence $m_1 \geq 2$. We now choose a subset D_2 of D such that $|D_2| = |D| - k > 0$. Let

$$G^* = G - \{u_0x : x \in D_2\} + \{bc : b \in B, c \in C \setminus \{u_0\}\} + \{pq : p \in D, c \in A\}.$$

It is routine to check that $G^* \in \mathcal{C}_{n,s}$ with bipartition (X, Y) . We claim that $EE(G) < EE(G^*)$.

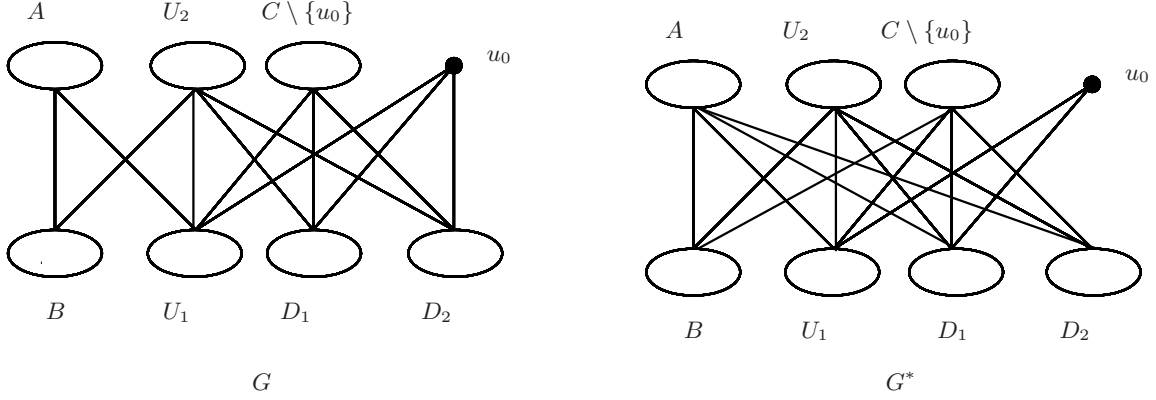


Figure 3. G^* and G^{**}

We color the edges u_0x blue if $x \in D_2$ and red if $x \in U_1 \cup D_1$. For any $k > 0$ and $W \in W_{2k}(G)$, let $\Psi(W)$ be the closed walk of length $2k$ that is obtained by changing all the blue edges u_0x to ax and all the red edges u_0y which is incident with a red edge to ay , where a is a vertex of A . It is obvious that $\Psi(W) \in W_{2k}(G^*)$ and Ψ is an injection. Hence we have for any $k > 0$, $M_{2k} \leq M_{2k}(G^*)$. Together with $M_{2k-1} = M_{2k-1}(G^*) = 0$, we get $EE(G) \leq EE(G^*)$. Furthermore, as $M_2(G) = |E(G)| < |E(G^*)|$, we know that $EE(G) < EE(G^*)$. So, we get our conclusion. ■

Theorem 4.5 *The unique graph in $\mathcal{C}_{n,s}$ with the maximum Estrada index is $O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - s})$.*

Proof. Let G be a graph with the maximum Estrada index in $\mathcal{C}_{s,n}$. Let U be a vertex cut of G containing s vertices. we distinguish the following two cases:

Case 1. All the components of $G - U$ are singletons. In this case, we have $G = K_{s,n-s}$. For $s = \lceil \frac{n-1}{2} \rceil$, it is nothing to say since $K_{s,n-s} \cong O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - s})$. For $1 \leq s \leq \lceil \frac{n-1}{2} \rceil - 1$, by Lemma 4.3, $EE(K_{s,n-s}) < EE(O_s \vee_1 (K_1 \cup K_{n-s-2,1}))$, which contradicts the maximality of G .

Case 2. One component of $G - U$, say G_1 , contains at least two vertices. By Lemma 4.4, we know that $G - U$ has exactly two components G_1 and G_2 , with $G_2 \cong K_1$. Therefore, there exist p, q with $p + q + s + 1 = n, p \geq s, q > 0$, such that $G \cong O_s \vee_1 (K_1 \cup K_{p,q})$. Then by Lemma 4.1 and Lemma 4.2, we have $q + s \leq p \leq q + s + 1, p + q + s + 1 = n$. Hence we have $p = \lfloor \frac{n-1}{2} \rfloor$, i.e., $G \cong O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - s})$. This completes the proof. ■

Corollary 4.6 *Let $\mathcal{D}_{n,s}$ be the set of graphs with n vertices and edge-connectivity s . One has that the unique graph in $\mathcal{D}_{n,s}$ with the maximum Estrada index is $O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - s})$.*

Proof. As is well known [1] that $\kappa(G) \leq \kappa'(G)$, hence for any $G \in \mathcal{D}_{n,s}$ there exists $k \leq s$ such that $G \in \mathcal{C}_{n,k}$. Then by Theorem 4.5, we have $EE(G) \leq EE(O_k \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - k}))$. On the other hand, $O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - s}) \in \mathcal{D}_{n,s}$ and $O_k \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - k}) \subset O_s \vee_1 (K_1 \cup K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil - s})$ as $k \leq s$, and hence we get our conclusion. ■

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